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Further Computations of the He Atom Ground State

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Abstract

Recently reported computations have been extended to give ten more decimals of accuracy in the ground state energy of the Schrodinger equation for the idealized Helium atom. With the F basis - Hylleraas coordinates with negative powers and a logarithm of s - carried to the fiftieth order (N = 24,099 terms) we find the eigenvalue
E = -2.90372 43770 34119 59831 11592 45194 40444 66969 25309 ...

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In a recently published paper [1], I reported the results of large scale systematic computations of the ground state eigenvalue of the Hamiltonian for the idealized Helium atom,

$$H = -\frac{1}{2}[\nabla_1^2 + \nabla_2^2] - 2/r_1 - 2/r_2 + 1/r_{12}, \qquad (0.1)$$

using the variational method with several basis sets formed with the Hylleraas coordinates,

$$s = r_1 + r_2, \quad t = r_1 - r_2, \quad u = r_{12} = |\vec{x}_1 - \vec{x}_2|. \qquad (0.2)$$

The most rapid convergence was found with the "F-Basis",

$$\psi = \sum C_{l,m,n} \, (1, lns) \, e^{-ks/2} \, s^l \, (u/s)^m \, (t/s)^n \qquad (0.3a)$$
$$l, m = 0, 1, 2, 3, \ldots, \quad n = 0, 2, 4, 6, \ldots \qquad (0.3b)$$

We designate a calculation of order ω to mean a basis set including all terms with $l + m + n \leq \omega$. Here, the scale parameter is fixed at $k = 2$.

The previous results went through $\omega = 37$; and now we report continued results through $\omega = 50$. The table below presents the new results, as a continuation of Table 2 in the previous publication. Also shown is the Ratio of successive differences which is one measure of convergence rate. Figure 1 in the previous paper showed a very rapid rise in the accuracy with increasing N, the number of basis functions used; and this new data shows no diminution of that rapid climb.

New Calculated Results with the F-Basis

ω	N	Energies	Ratios
36	9499	" 40438 342	3.11
37	10259	40444 00495	11.1
38	11057	40444 51579 435	3.81
39	11897	" 65044 4349	8.65
40	12779	66593 038	4.84
41	13703	66913 05205	6.81
42	14671	66960 00893 6	6.18
43	15683	66967 621	5.43
44	16741	66969 023	7.66
45	17845	66969 20593	4.44
46	18997	" 24711 8	9.00
47	20197	25170 030	3.75
48	21447	25292 13	9.10
49	22747	25305 571	3.14
50	24099	25309 838	

The ditto marks " in the table indicate that blocks of repeated digits have been left out, so that we can better see the new digits at each step.

With this data we can extrapolate to:

E* = -2.90372 43770 34119 59831 11592 45194 40444 66969 25310 5

References

[1] Charles Schwartz, "Experiment and Theory in Computations of the He Atom Ground State", *International Journal of Modern Physics E* **vol. 15, no. 4**, pp. 877-888 (2006). The original preprint is posted at the e-Print arXiv: physics/0208004 ; and some further information is available at http://socrates.berkeley.edu/∼schwrtz/physics.html